Towards Deriving Theories from Data: Frontiers for Model Inference in Astro-&Geophysics

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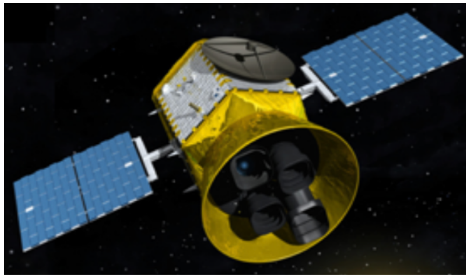
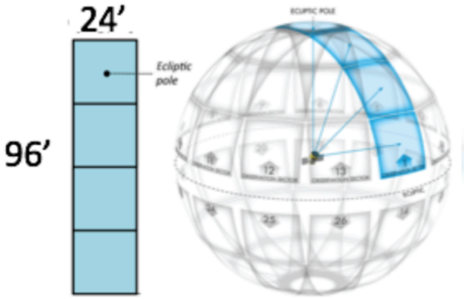
Overview

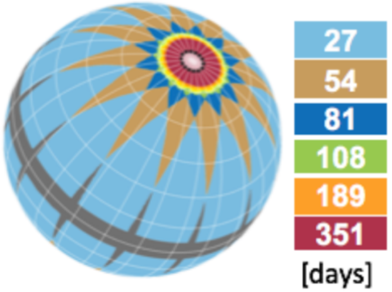
- Discuss AI in science – now and in the future
- Based on two examples:
  - Astrophysics: Exoplanet search
  - Geophysics: Earth deformation, volcanoes

Exoplanet Search





4x 2048x2048 CCDs



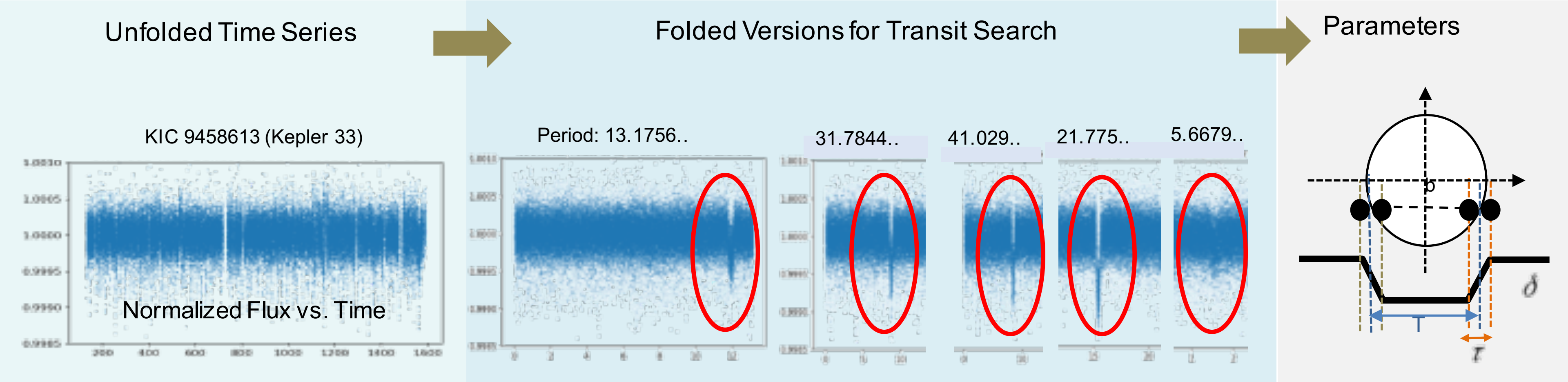
Transiting Exoplanet Survey Satellite (TESS)

- Near all-sky survey
- Launched April 18, 2018
- Kepler mission follow-up, stars 10-100 brighter
- Expecting thousands of new exoplanets smaller than Neptune and potentially dozens that are comparable to our Earth
- Full frame images every 30 minutes, 200,000 pre-selected stars monitored with 2 min cadence
- TESS processing pipeline extracts light curves
- Problems similar to future Big Data applications, e.g., Large Synoptic Survey Telescope (LSST) and others

[https://tess.mit.edu; https://tess.gsfc.nasa.gov; Ricker14]

Exoplanet Search

Transit Search: State-of-the-art



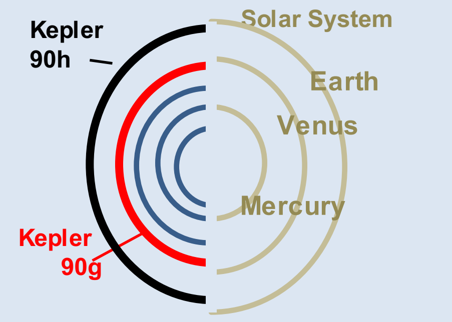
→ Machine learning and other methods typically applied on folded light curves [Shallue18]

[Kovacs02, Seager11, Winn14]

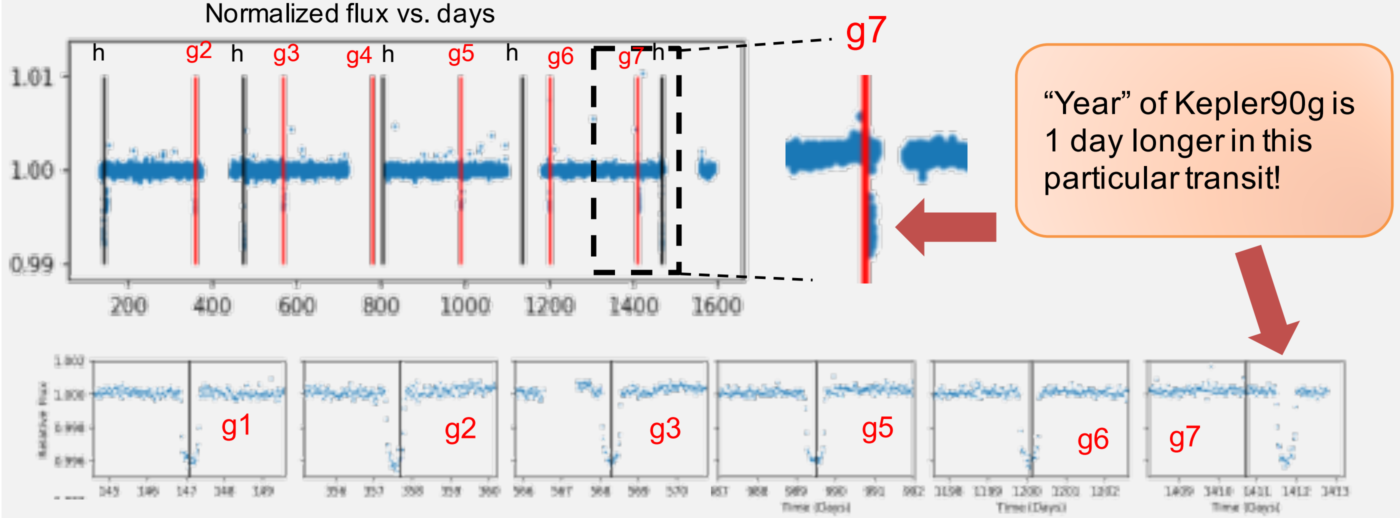
Exoplanet Search

However, there is more information in the unfolded time series.

→ Revealing irregular Transit Timing Variations (TTV) in Kepler90 system



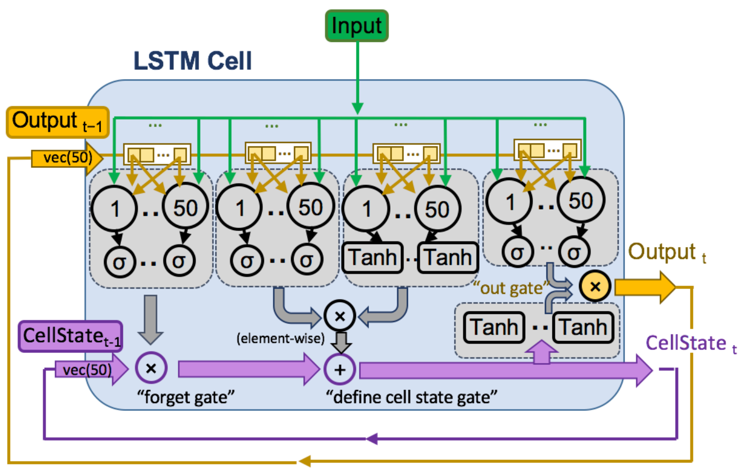
Period [days]	h: 331.6	g: 210.6
Mass [Jupiter Masses]	h: <1.2	g: <0.8

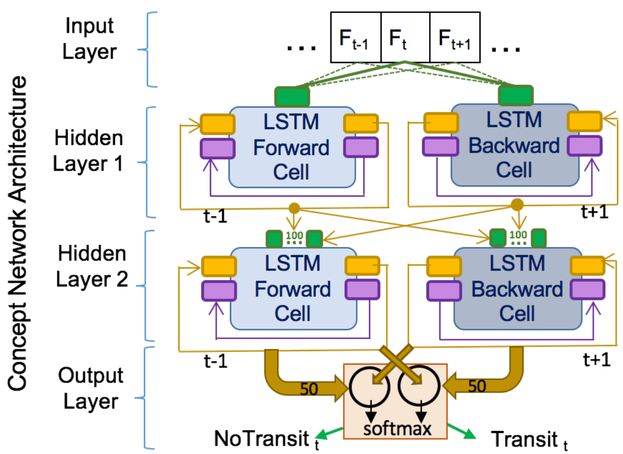


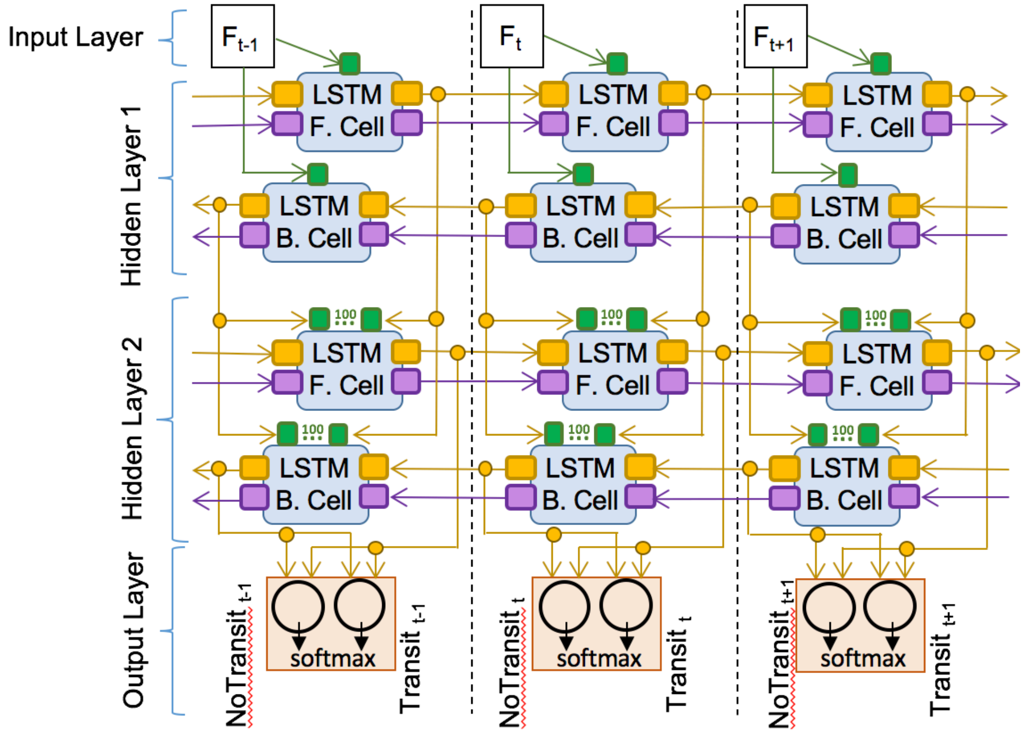
“Zooming” in on transits; red & black lines = catalog-listed periods

Bi-directional LSTM Networks in Exoplanet Search

A Toy Example:







Networks that are "deep" in time

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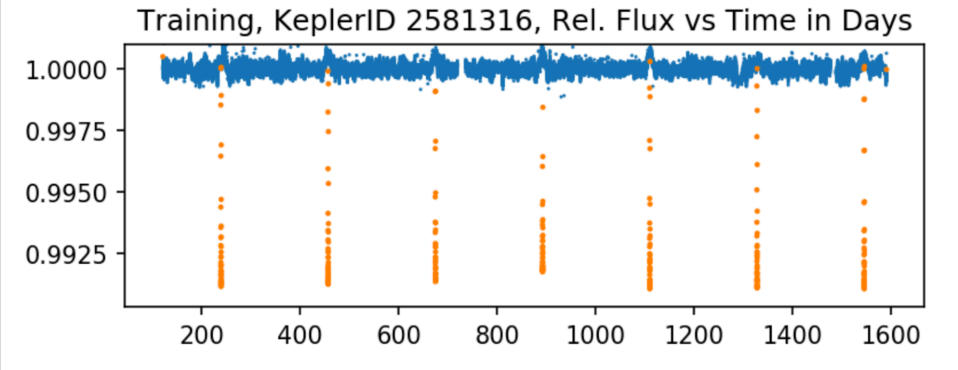
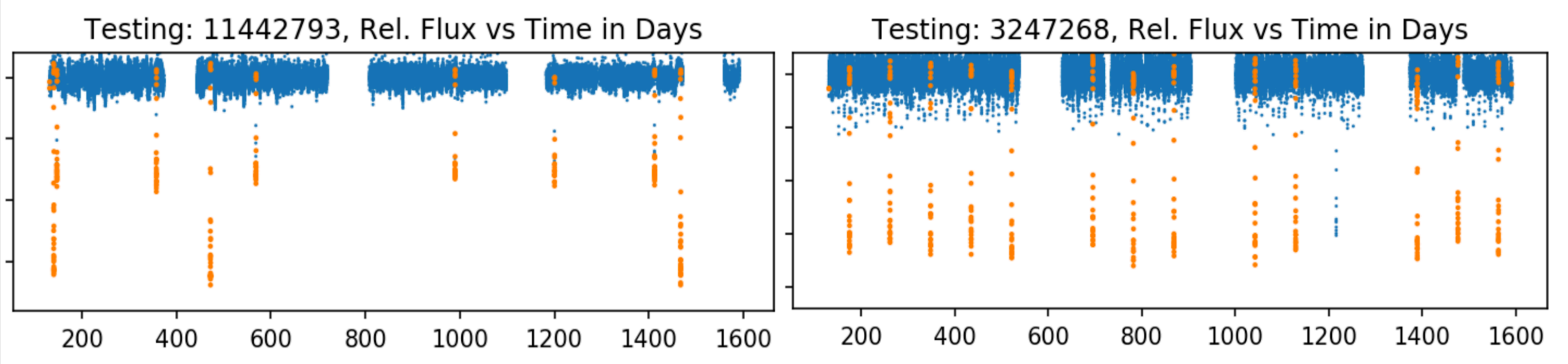
Bi-directional LSTM Networks in Exoplanet Search

BDLSTM example: learning **planet transits**



Applying trained BDLSTM to other light curves

[training: 50 epochs, 1 second steps, 0.5 dropout rate, until accuracy = 0.9797]



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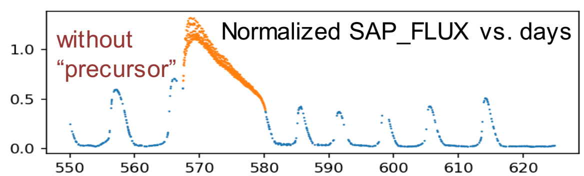
Bi-directional LSTM Networks: Other Phenomena

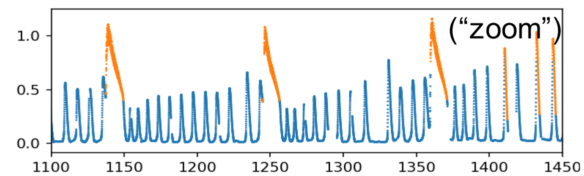
Variable Star Phenomena: **Learning Dwarf Nova Events**

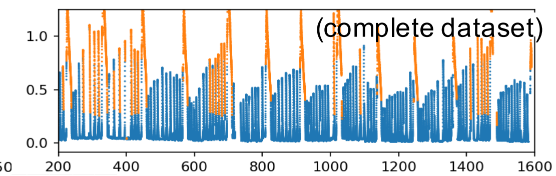
Example: V344 Lyr (Kepler 7659570)

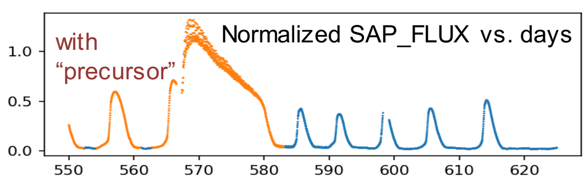
Training set = 1 piece of time series

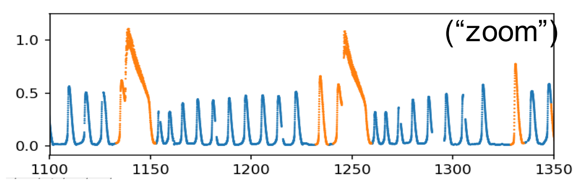
Preliminary BDLSTM Prediction on Test Set (rest of time series)

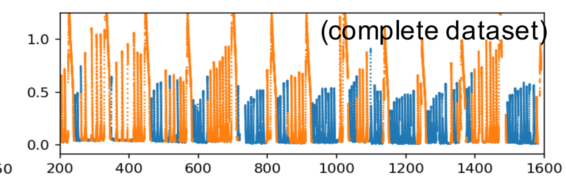












Note: potentially useful prediction capability based on empirically learned model

Next: Establishing Data – Model Connections

What do humans typically do?

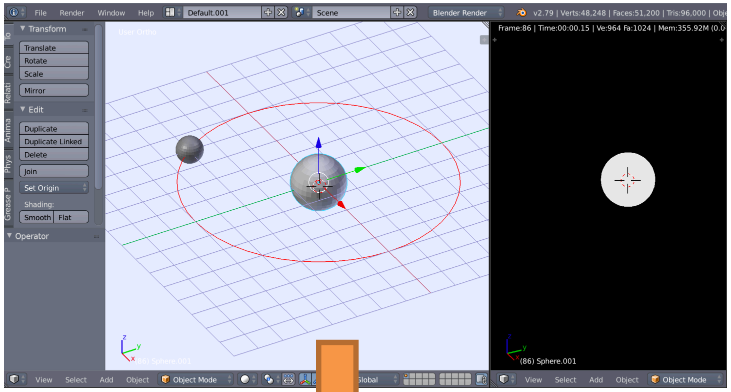
- Look at light curve → develop a "mental model" (hypothesized planetary system, related phenomenon)
- "Play" in imagination, unfold over time
- Anticipate dynamics
- Look back at the light curve for supportive clues

→Inverse problem solved iteratively by generating multiple forward models + pruning those that do not exhibit the right properties

→This process can be automated

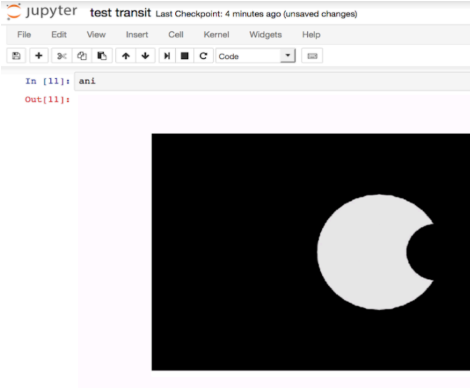
Next: Establishing Data – Model Connections

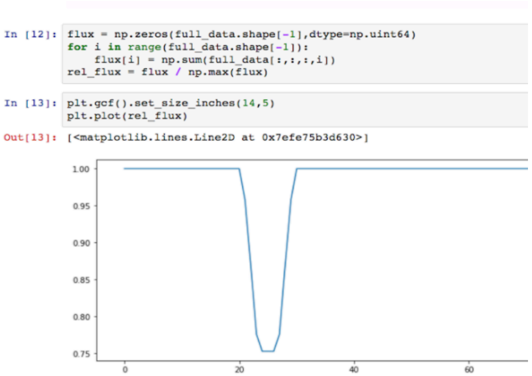
Proof of concept example:

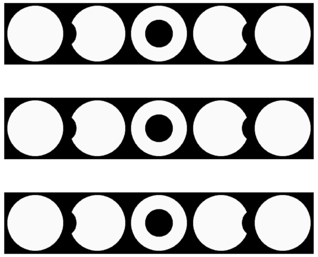


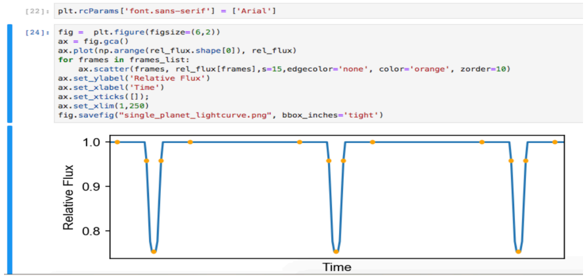
blender.org Raytracer

Programmatic Interface in Python Jupyter Notebooks









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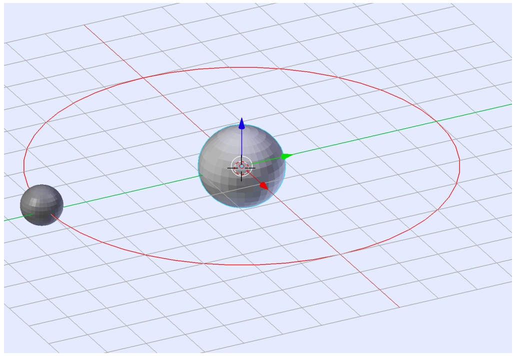
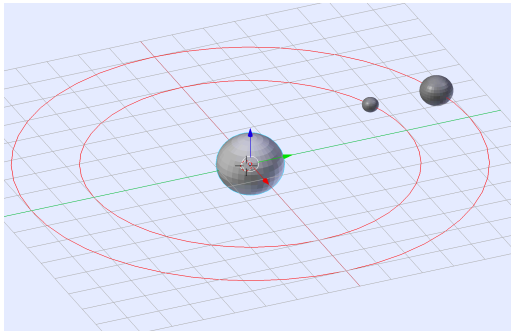
Generative Approach

Generate Physical Model

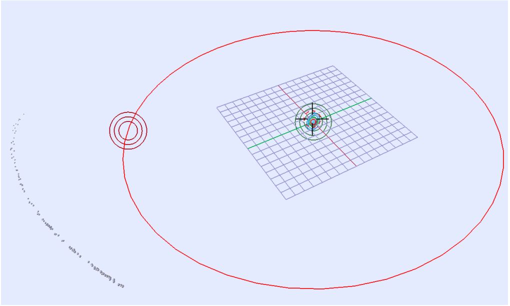
Scenario: One planet



Scenario: Two planets



Scenario: Irregular Orbiting Debris



Generative Approach: One Planet

Theoretical Domain

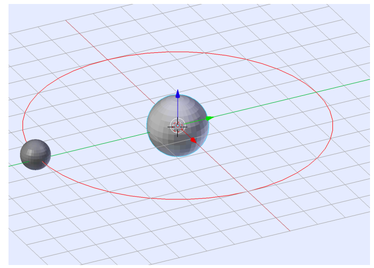
Physics

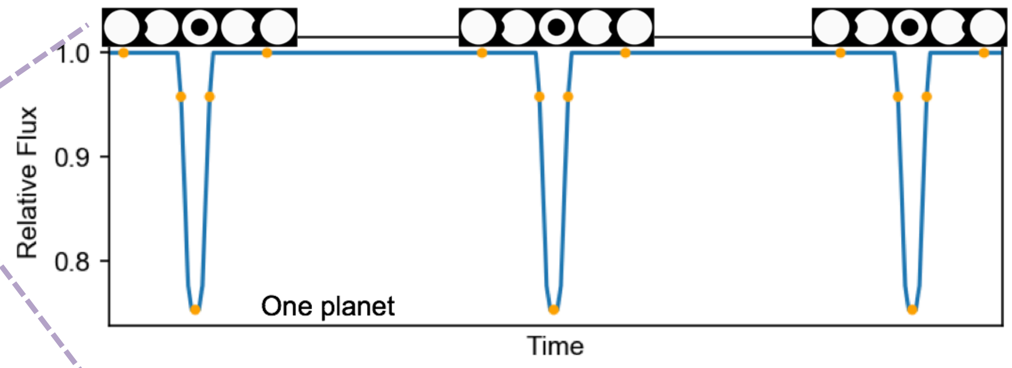
Model Features

Data Features

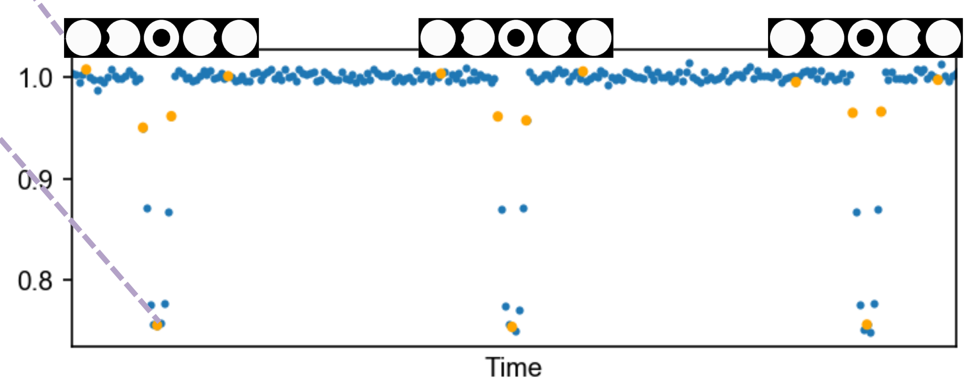
Empirical Domain

A “Rosetta Stone” linking models & theories to data

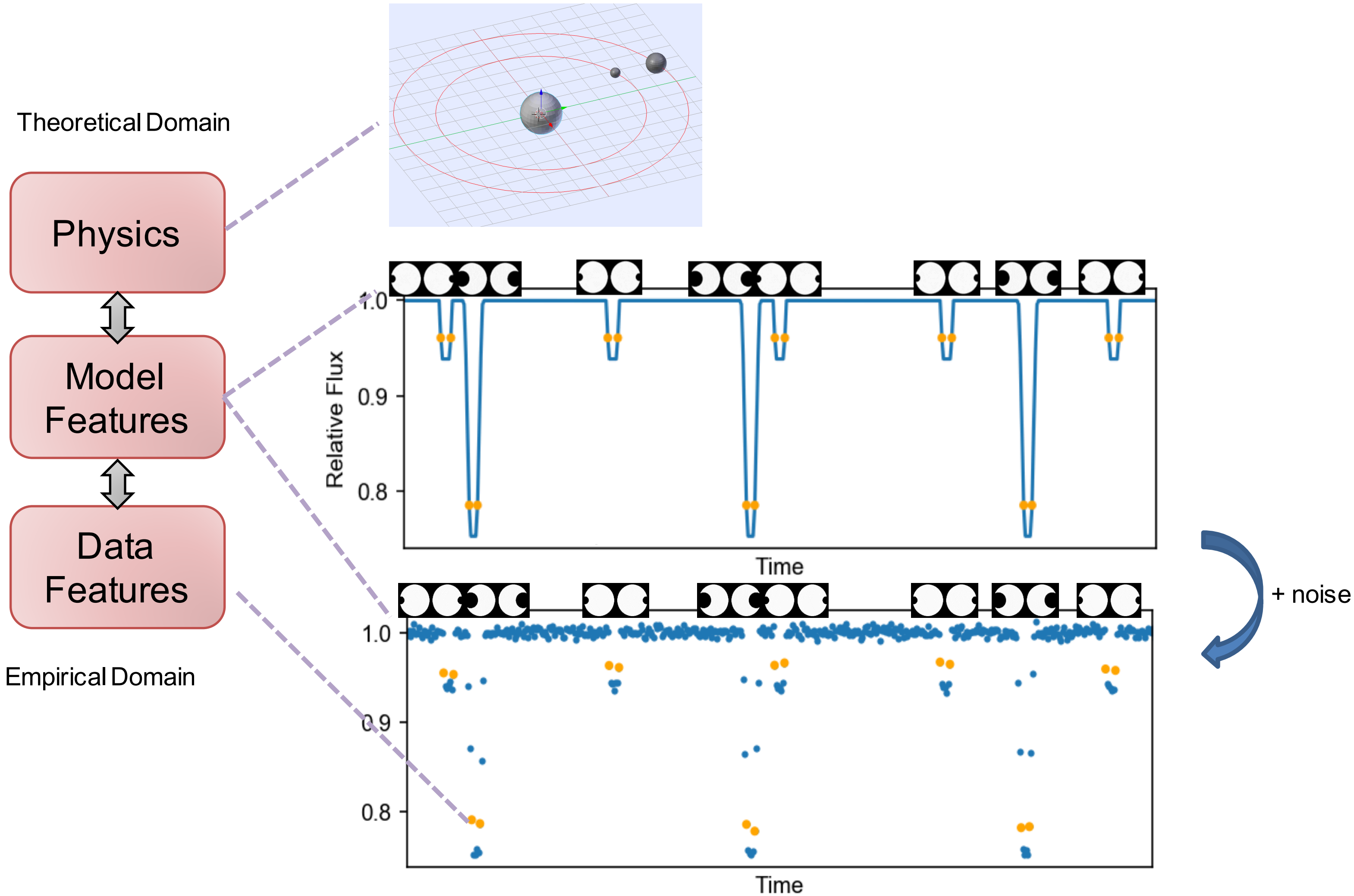




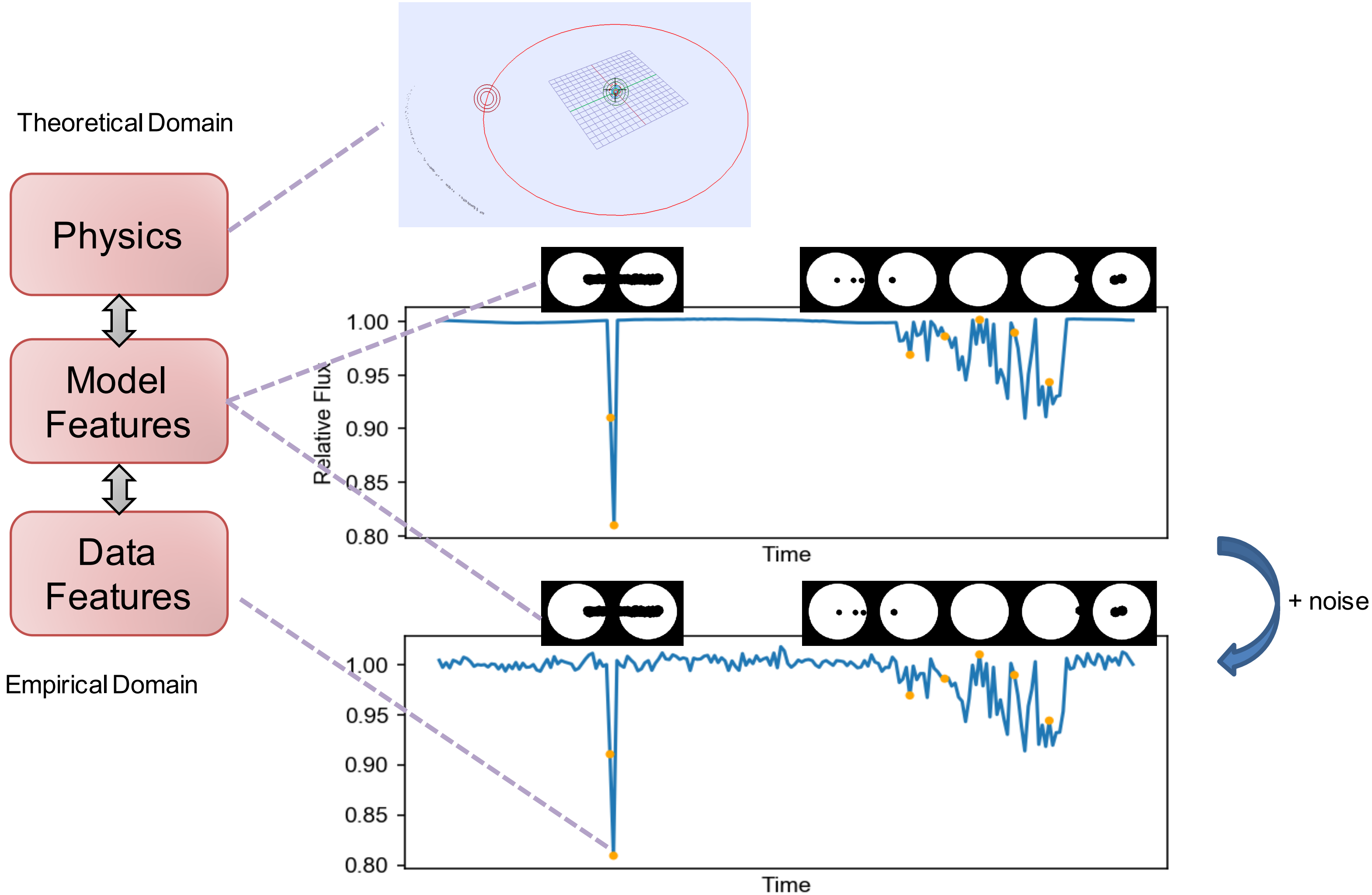
+ noise



Generative Approach: Two Planets

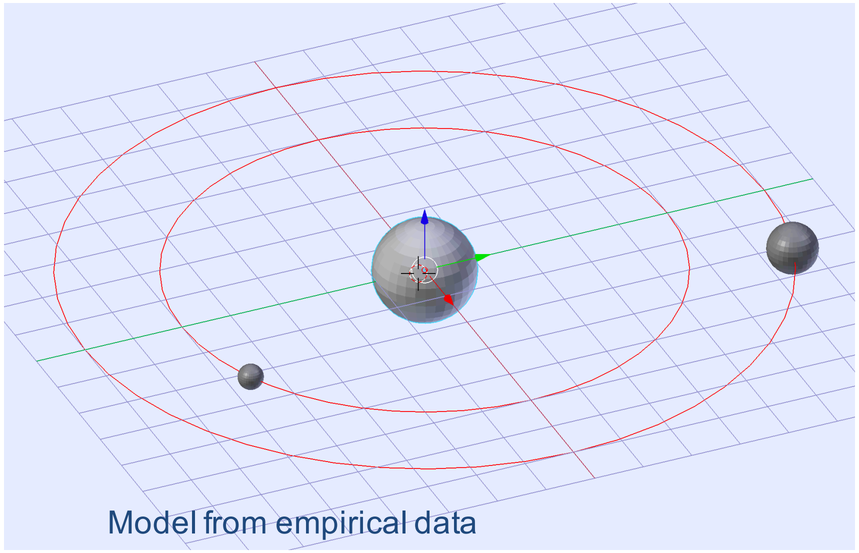


Generative Approach: Irregular Debris



Adding Inference Capabilities

A system with a confirmed planet might have other planets, moons, debris disks, …



→ create an “autocomplete” capability (inference engine) for planetary systems

Adding Inference Capabilities

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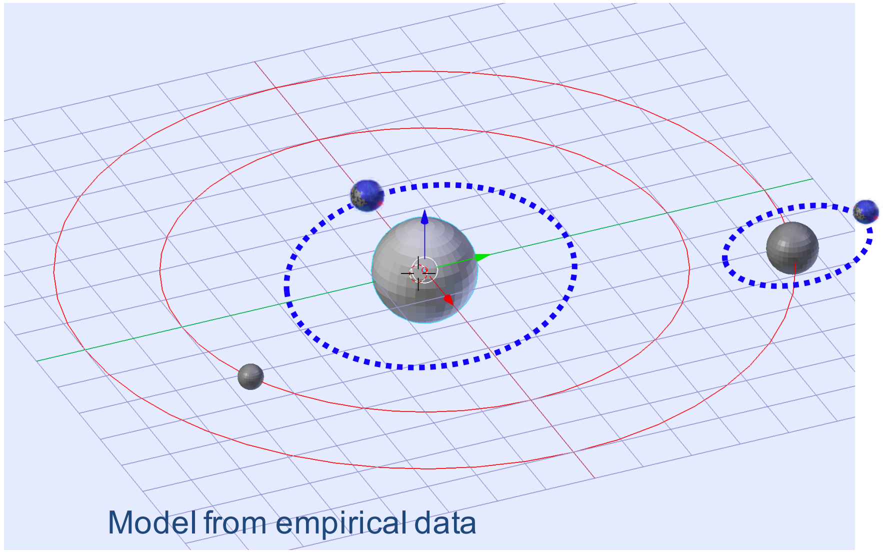


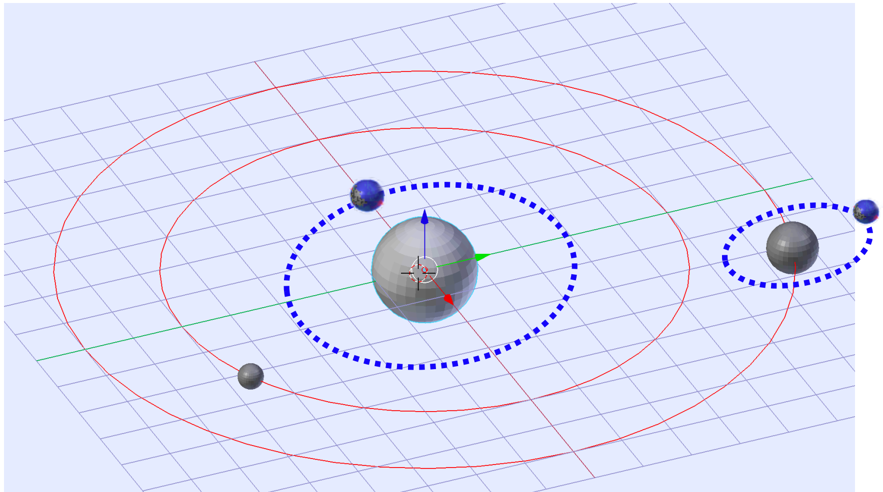
Model from empirical data

→ create an “autocomplete” capability (inference engine) for planetary systems

→ “Guess where & what” with plausible physics

Adding Inference Capabilities

A system with a confirmed planet might have other planets, moons, debris disks, …



Model from empirical data

→ create an “autocomplete” capability (inference engine) for planetary systems

→ “Guess where & what” with plausible physics

→ Create a population of forward models and plausible variants (e.g., using genetic programming)

Derive empirical features to look for, if models were describing reality

- Generate neural networks that have higher attention in those areas
- Test / falsify multiple theories in parallel

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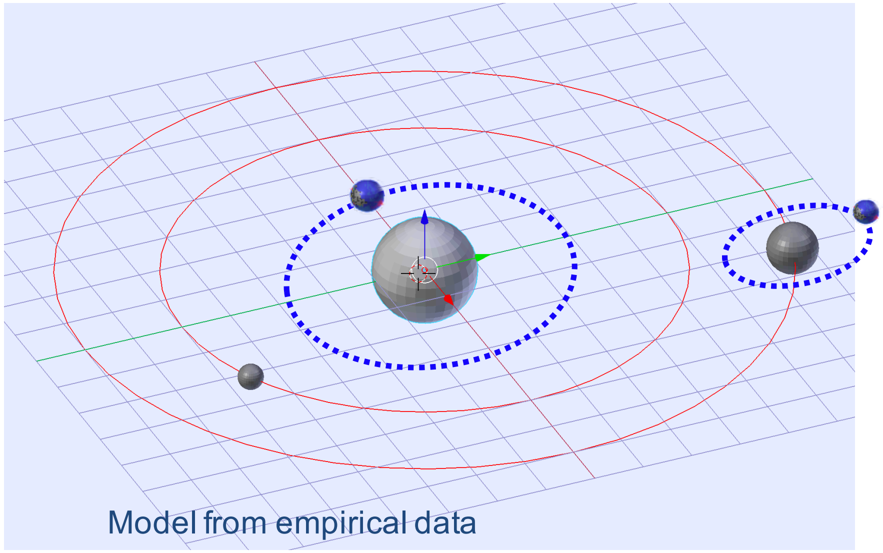
Adding Inference Capabilities



Generative approach facilitates inference on other properties

Planet mass, radius, orbital parameters, rotation rate, obliquity
⇒ gravitational acceleration
⇒ atmosphere parameters
⇒ potential mean density/rockiness
⇒ inferences on core, magnetosphere.

Planet surface temperature
⇒ greenhouse warming
⇒ thermal emission
⇒ atmospheric gases and compositions.

Spectroscopy parameters
⇒ biosignatures, gases
⇒ indicator factors of habitability

Host star properties
⇒ luminosity/temperature, spectral type, activity, rotation rate, and flare activity
⇒ habitability

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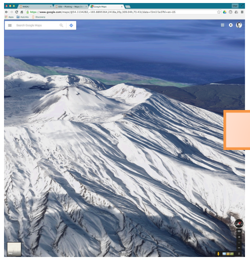
Can this approach can be transferred to other domains?

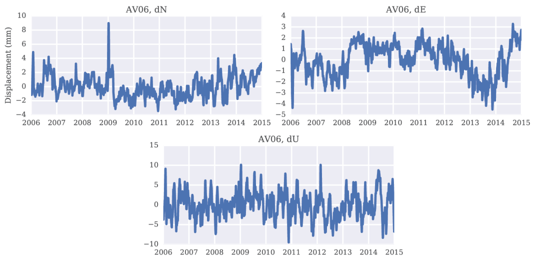
Geophysics Example

Volcanology

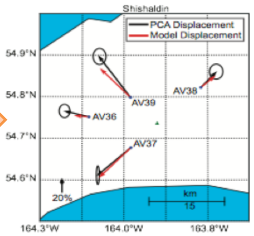
GPS Sensors



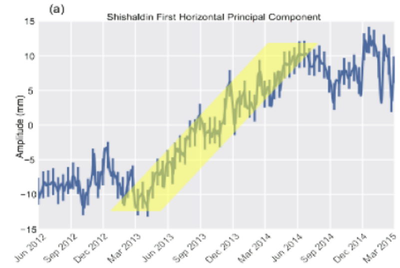
Time Series



Empirical Model

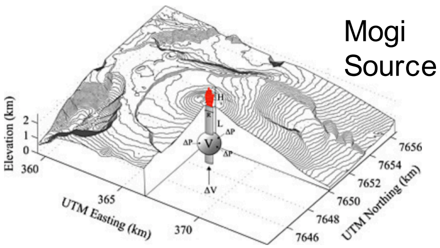


Classifier for
Earth deformation/ inflation event



Theoretical Model

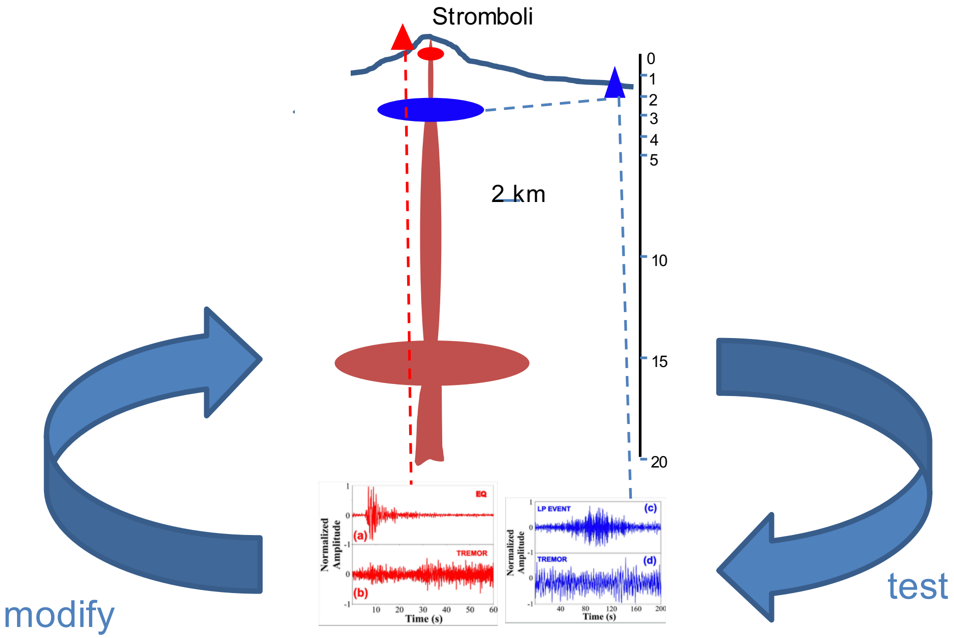
Mogi
Source



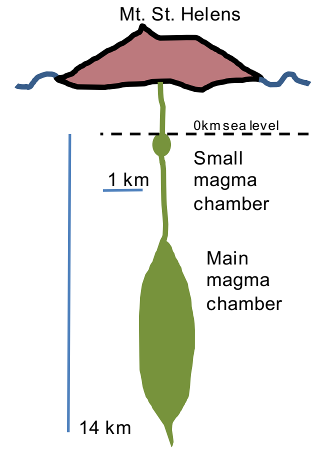
[J.Li, C.Rude, D.Blair, M.Gowanlock, T.Herring, V.Pankratius. Journal of Volcanology and Geothermal Research, 2016]

[Hibert et al., GRL ‘15]

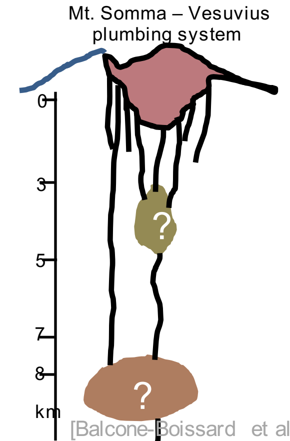
Inferring Models at Higher Abstraction Levels



[Giovanetti et al. Remote Sens., 8(4), 2016, Fig 3]



[Earle, Physical Geology, 2015, Fig. 4.12]

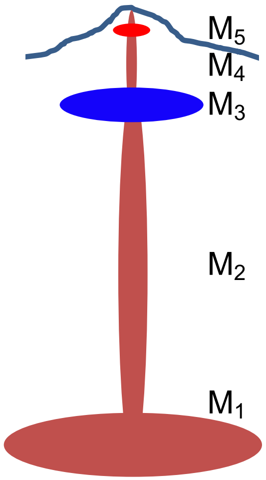


[Balcone-Boissard et al., Nature Scientific Reports 6, 21726, 2016; Fig. 1]

AI Theorem Prover for Science Models / Test Case Generator for Empirically Observable Features

- Derive test cases: “this property should be observable if this model was right”
- Derive falsification cases: “property that should never be observed if this model was right”
- Derive invariants: “this predicate should always be true if this model was right”

Symbolic Model Manipulation: Algebraic Approach



$$M_{seed} = M_1 \oplus M_2 \oplus M_3 \oplus M_4 \oplus M_5$$

perturb

$$\begin{aligned}\mathfrak{P}(M_{seed}) &= \mathfrak{P}(M_1 \oplus M_2 \oplus M_3 \oplus M_4 \oplus M_5) \\ &= \mathfrak{P}(M_1) \oplus \mathfrak{P}(M_2) \oplus \mathfrak{P}(M_3) \oplus \mathfrak{P}(M_4) \oplus \mathfrak{P}(M_5)\end{aligned}$$

M_i includes info on
- variables
- dom(variables)
- constraints(variables)

$$M_{1_1} \dots M_{1_n}$$

trim

$$\begin{aligned}\mathfrak{T}(M_{seed}) &= \mathfrak{T}(M_1 \oplus M_2 \oplus M_3 \oplus M_4 \oplus M_5) \\ &= M_1 \oplus M_2 \oplus M_3 \oplus M_4\end{aligned}$$

extend

$$\begin{aligned}\mathfrak{E}(M_{seed}, M_6) &= \mathfrak{E}(M_1 \oplus M_2 \oplus M_3 \oplus M_4 \oplus M_5; M_6) \\ &= M_1 \oplus M_2 \oplus M_3 \oplus M_4 \oplus M_5 \oplus M_6\end{aligned}$$

generate

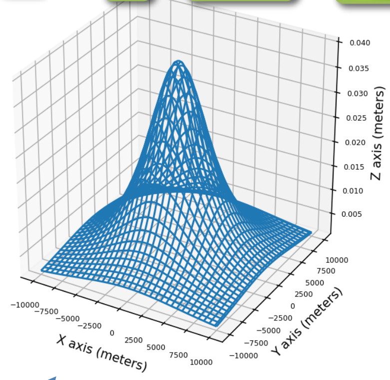
$$\mathfrak{G}(space(M)) = M_i \text{ with } M_i \in space(M)$$

Remark: more elaborate modeling requires introduction of a type system, constraints / domain-specific rules, …

[Pankratius et al., AGU'18]

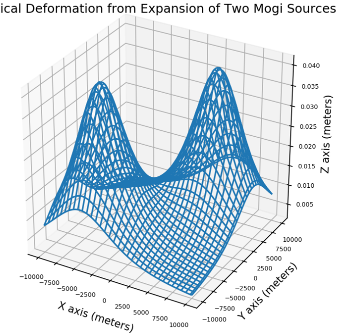
Examples for M_i in Geoscience

Mogi
Source Pos X
Source Pos Y
Source Depth
Amplitude
0
0
5km
1E6



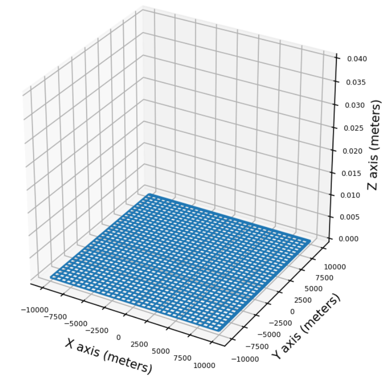
Composite
Mogi 1
Mogi 2
. . .
. . .

Vertical Deformation from Expansion of Two Mogi Sources

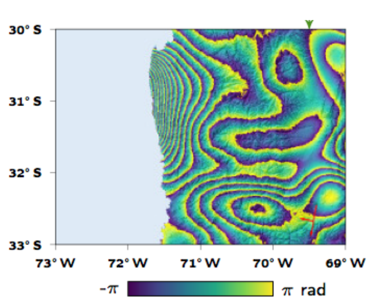


$\emptyset$

No deformation



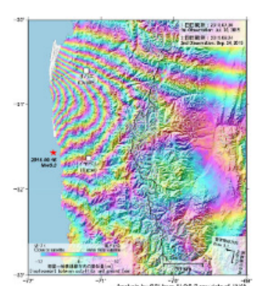
Compute Interferogram



add machine-learned noise components

Test with Reality

Compare with real-world InSAR satellite or UAV interferogram



Genetic Programming in Python, with a scikit-learn inspired API:

gplearn

```
est_gp = SymbolicRegressor(population_size=2000,
                           generations=20, stopping_criteria=1e-6,
                           model_set = model_set_minimal, const_dict=constants_dict,
                           p_crossover=0.1, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.5,
                           max_samples=0.3, verbose=1,
                           parsimony_coefficient=0.0, random_state=2,
                           function_set=function_set, metric='rmse')
```

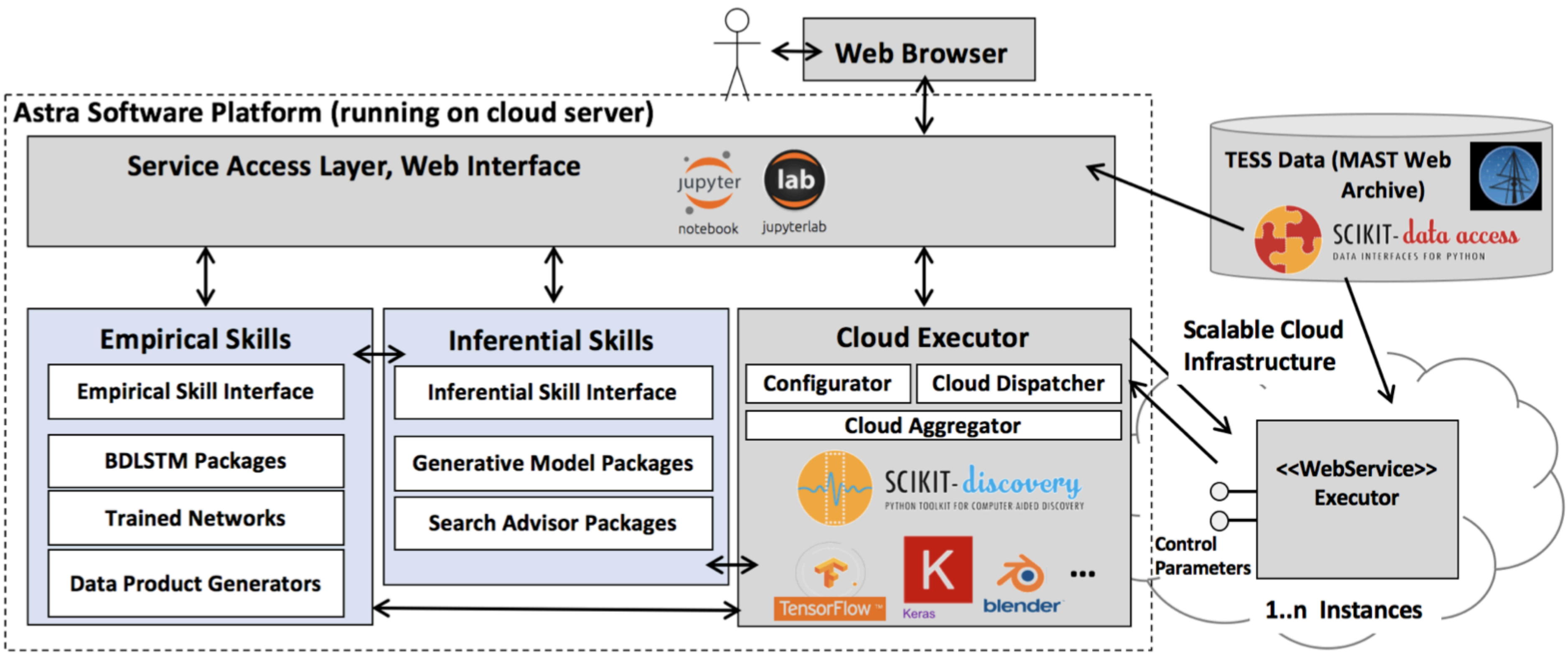
```
est_gp.fit(inputs,raveled_results);
```

```
    |    Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    29.29   0.379876288789        7 0.00520790406466 0.00505486366858      5.84m
   1      7.8   0.030539641708        7 0.00414515971233  0.0041535007502      3.94m
   2     7.47  0.0217428270721        7 0.00395724793119 0.00393784066313      3.10m
   3     7.54  0.0211037854184        7 0.00318999426958 0.00317289165736      2.65m
   4     7.46  0.0220503883175        7 0.00230268888262 0.00238928755349      2.32m
   5      7.4  0.0254420907836        7 0.00221451369295 0.00221619043055      2.07m
   6     7.56  0.0264524039272        7 0.00137761712883 0.00141688526414      1.85m
   7     7.58  0.0268504367133        7 0.00115849684897 0.00117389812701      1.67m
   8     7.38  0.0223381746746        7 0.00115217180138 0.00117656259719      1.50m
   9     7.56  0.0251189315923        7 0.00108114916971 0.00108388332304      1.34m
  10     7.34  0.0164327114159        7 0.00106194685183 0.00109198779104      1.18m
  11     7.48  0.0219102240383        7 0.000698760418825 0.000708090443757      1.04m
  12     7.43  0.0224319079123        7 0.000695351954025 0.000709526792845     53.96s
  13     7.56  0.0260644565465        7 0.000680539227613 0.000715654687798     45.86s
  14     7.42  0.0224007926631        7 0.000672186500833 0.000688974221301     37.89s
  15      7.4  0.0189147300504        7 0.000659537013899 0.000655411966447     30.09s
  16     7.44   0.020894681919        7 0.000648583111273 0.00066007953655     22.42s
  17     7.44  0.0209206195977        7 0.00064154116245 0.000663021882061     14.85s
  18     7.29  0.0159319391861        7 0.000638331590463 0.000664348006707      7.38s
  19     7.52  0.0192420494408        7 0.000637164640365 0.000659453373537      0.00s
```

[Rude, Pankratius, Rongier: work in progress]

- Where do we go from here?

Blueprint for "Astra"
An AI Science Assistant with Domain Knowledge



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Conclusion

- Big Data & instrument fusion in scientific applications
  → push for more automation at all levels
- We need to rethink automation in the scientific process
- Problems go beyond detection, classifications, statistics
- Automated insight generation will be key
- Vision for future:
  AI science assistants that have domain knowledge

Thanks!

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